Scalable Solvers for 3D Extended Magnetohydrodynamics

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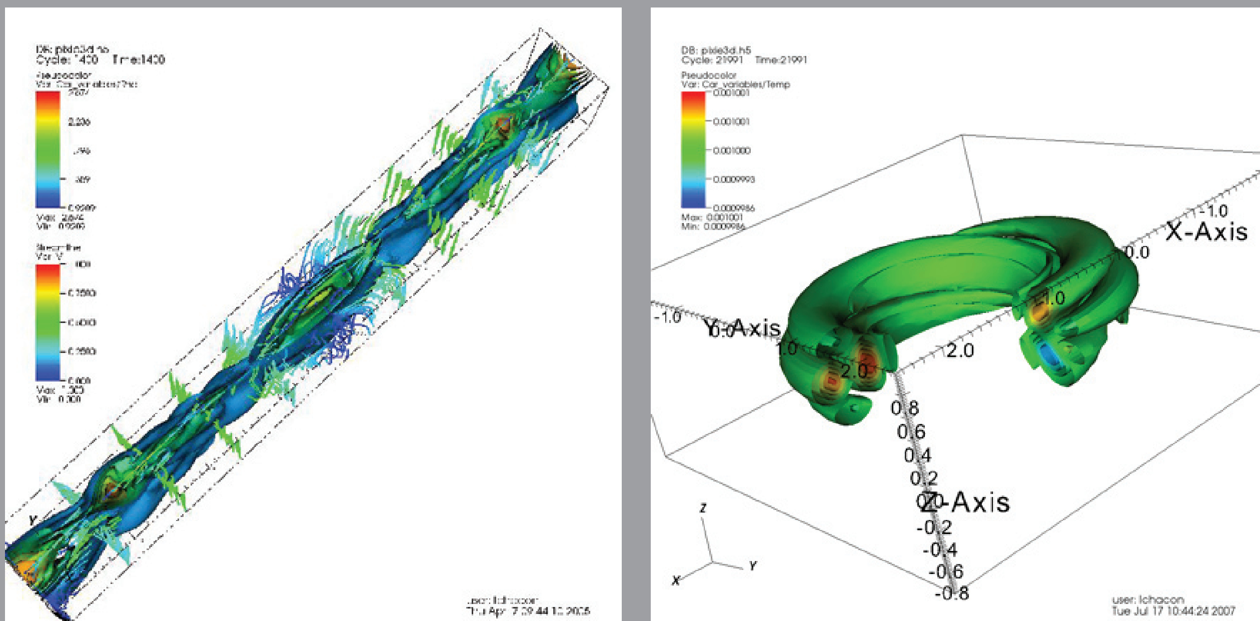

Fig. 1. Sample 3D simulations with PIXIE3D, a fully implicit extended MHD simulation code. The left figure depicts densities and velocities in the nonlinear stage of a 3D Kelvin-Helmholtz unstable configuration with differential rotation. The figure on the right depicts temperature during the evolution of a helical perturbation in a 3D toroidal fusion device.

Extended magnetohydrodynamics (XMHD) is a highly coupled, nonlinear partial differential equation system characterized by multiple physical phenomena that span a very large range of length and time scales. Numerically, XMHD results in very ill-conditioned algebraic systems, which require implicit time stepping for efficiency, and spatial adaptivity to resolve dynamically forming thin layers. We summarize our progress towards fully implicit 3D XMHD using Newton-Krylov methods, and towards the implementation of fully implicit adaptive mesh refinement (AMR).

The purpose of this project is to explore efficient time integration algorithms for XMHD. XMHD describes processes occurring in plasmas, which are common in the natural world, and are highly important for many advanced DOE applications. The predictive simulation of plasmas is a crucial capability, one that requires the solution of strongly coupled equations on high resolution, adaptive meshes. Temporally, XMHD supports multiple, disparate time scales in the form of normal modes (waves). These waves are generally much faster than the slow dynamical time scales of interest. Explicit techniques are unsuitable for XMHD, as they must resolve the fastest supported time scale. Semi-implicit methods can effectively step over explicit time-step constraints, but concern exists about their accuracy for large time steps [1]. Implicit methods, however, can step over fast time scales to accurately resolve the dynamical time scale [2], but a large-scale system of stiff nonlinear equations must be solved every time step. For this, robust and efficient parallel iterative solvers are necessary. Our work focuses on the development of scalable, fully coupled Newton-Krylov-based (NK) solvers for XMHD.

Preconditioning is key to accelerating NK. Formulating suitable preconditioning strategies for XMHD is a main goal of this project. We aim at enabling the use of multi-level techniques in the preconditioning stage, because they have the potential of delivering optimal convergence rates with problem size [3,4,5]. In this regard, we have pioneered the “physics-based” preconditioning concept. At the heart of the approach is the “parabolization” of the hyperbolic XMHD system, which recovers block diagonal dominance and renders XMHD multilevel-friendly. Sample results of an XMHD grid convergence study showing the excellent algorithmic performance of the approach are given in Table 1. In particular, note that the CPU is proportional to the number of mesh points, and the number of GMRES iterations is not only bounded, but improves under grid refinement.

Table 1. XMHD grid convergence study

1 time step, $\Delta t = 1.0$, V(3,3) cycles, mg_tol=1e-2

Grid	GMRES/Δt	CPU_{exp}/CPU	$\Delta t/\Delta t_{exp}$
32x32	22	0.44	110
64x64	12	1.4	238
128x128	8	6.2	640
256x256	7	30	3012

We have implemented these developments in a 3D XMHD simulation tool, PIXIE3D [6]. PIXIE3D features a conservative, solenoidal finite-volume discretization in general curvilinear geometry, with remarkable stability properties. Sample PIXIE3D results are depicted in Fig. 1.

Table 2. Implicit AMR grid convergence study.

$\Delta t = 1$ (fixed), $\eta_k = 0.1$, $\epsilon_{rel} = \epsilon_{abs} = 10^{-7}$, 2 SI iterations, V(3,3) cycles

	GMRES its/Δt				
Levels	1	2	3	4	5
32×32	3.4	7.9	12.0	19.3	33.7
64×64	6.5	11.7	19.1	33.2	–
128×128	12.5	20.1	27.2	–	–
256×256	19.9	27.5	–	–	–
512×512	26.3	–	–	–	–

Despite the efficiency benefits of a fully implicit temporal integration of XMHD, implicit time stepping alone is not sufficient for a truly optimal algorithm. Disparate length scales in XMHD result in dynamically evolving thin structures, which need to be resolved as the simulation proceeds. Using uniform grids for this purpose would result in unnecessarily large problems. In order to minimize the number of degrees of freedom required for a given simulation, grid adaptation is required. However, the integration of AMR and fully implicit time stepping is a challenging task. We have addressed this challenge by coupling physics-based preconditioned NK with structured adaptive mesh refinement (SAMR, provided by the SAMRAI package). We have developed an implicit AMR capability on 2D reduced MHD [7], which has demonstrated excellent algorithmic performance (Table 2). A calculation of a tilt instability using implicit AMR is shown in Fig. 2.

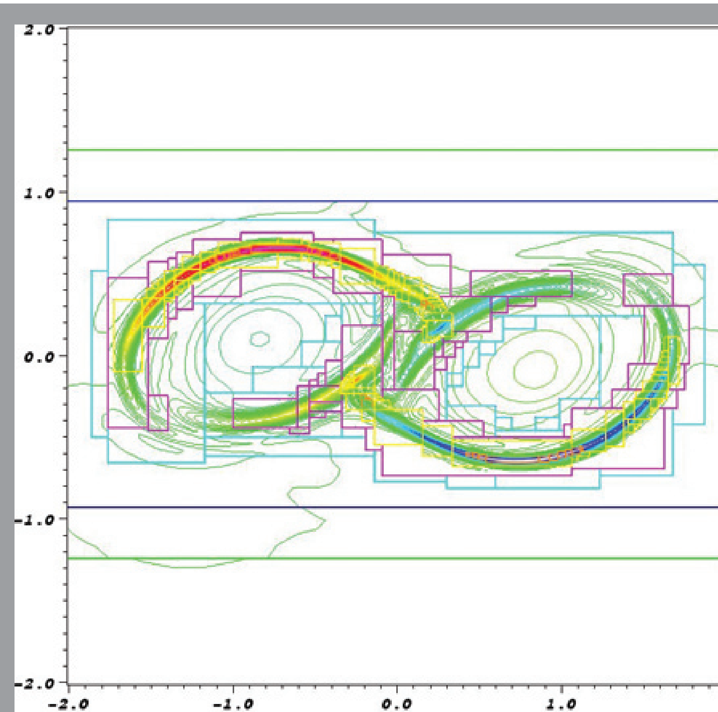

Fig. 2. Tilt instability calculation using implicit AMR.

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